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Transfer Operator Framework for Earth System Predictability and Water Cycle Extremes

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Focal Areas:

Ultimately, transfer operators provide a novel framework for predicting complex, partially-observed dynamical systems like the Earth System (focal area 2). In addition, transfer operators provide physics-based representation learning methods for data-driven analysis and prediction of coherent structures, like extreme events of the water cycle (focal area 3).

Science Challenge:

For chaotic dynamical systems, nonlinear instabilities lead to exponentially divergent trajectories in the evolution of system states. Unless a simulation is initialized with an infinite-precision snapshot of the state of the true system and all known physical effects that go into its evolution are directly computed, the future state predicted by the simulation will quickly diverge from that of the true system. Moreover, the Earth system is highly structured and contains localized coherent structures that are particularly important to predict. Predicting extreme events associated with coherent structures, like hurricanes and blocking events, is crucial for understanding the effects of global warming on the water cycle.

Rationale:

Whereas physics-based simulations like E3SM evolve individual states of a dynamical system, transfer operators [1] instead act on functions of the system state, known as *observables*. No matter how chaotic the underlying system, the evolution of system observables governed by transfer operators is always linear. But this comes at the cost of infinite-dimensional operators, since they act on all possible observables. Recent advances in machine learning have enabled sophisticated inference methods for finite-dimensional approximations of transfer operators that have shown great promise for predicting complex nonlinear systems.

Compared to the simulation-based approach, transfer operator methods more directly correspond to the realities of predicting the actual Earth system. The instrumental measurements through which we can access glimpses of the true Earth system state are, in fact, observables whose true evolution is governed by transfer operators. Effects of unobserved degrees of freedom must be explicitly parameterized in simulations, whereas transfer operator methods implicitly account for these effects. The implicit representations of transfer operators make them similarly well-suited to identify coherent structures with complex geometries. Implicit representations may be learned from data, without the need to fit to an explicit representational basis like wavelets or Fourier modes [2].

Narrative:

A system observable is a bounded function of the state of a dynamical system. As mentioned, the output of a measurement device is an observable of the underlying system. The Koopman operator [3] U^t governs the evolution of *all* such observables f and is defined via composition with the flow map Φ^t of the dynamical system: $U^t f = f \circ \Phi^t$. That is, if we take a measurement of, say, temperature at a certain point and then want to know the value of a temperature there at a later time t we can either let the system evolve under Φ^t then take the measurement after time t, or we can apply the Koopman operator to get the time-shifted observable $U^t f$. Thus the ground-truth for the prediction of any system observable is given by the action of the true (infinite-dimensional) Koopman operator. This includes the values of all instrument readings, as well as the value of the full Earth system state itself--known as the "full-state observable". In the probabilistic setting, Koopman observables become random variables that are distributed according to densities whose evolution is governed by the Perron-Frobenius operator. Because these transfer operators are adjoints, it is not necessary to distinguish between them [4].

A formal statement of the prediction problem for the Earth system can be stated as follows. Let X be the vector-valued Koopman observable that represents the collection of all measurements made of the Earth system, through e.g. the Global Observing System. Similarly, let Y represent the "observables of interest" that we wish to predict. Define the target function F_t to be the map from the history of observations X to the future value of Y out to lead time t. As stated above, the true value of Y at the future time t is given in terms of the Koopman operator as $U^t Y$.

The prediction problem then is to minimize $\|F_t \circ X - U^t Y\|$ [5].

Stated this way, the prediction problem encompasses many types of predictive models. These include statistical models like (N)ARIMA(X) [6], as well as analog forecasting methods from nonlinear dynamics [5], [7]. The kernel analog forecasting method has shown promising results for Earth system predictability [8]. This of course also includes predictive models based on direct, finite-dimensional approximations of transfer operators [4]. Linear Inverse Modeling is a common approach in climate science, and is equivalent to the linear transfer operator approximation method known as Dynamic Mode Decomposition [9]. More sophisticated nonlinear approximation methods have not been widely employed from Earth system prediction. Notably, because neural networks are universal function approximators, they can be trained to approximate the target function F_t [10].

There is a long way to go to scale up the transfer operator paradigm to the scale of Earth system models. Transfer operators however can also be used in conjunction with existing simulation models like E3SM.

One interesting possibility for improved mid-term prediction is to use transfer operators to predict (ensembles of) instrument readings and assimilate ESM runs to those predictions. This will incorporate observed data from the true system into predictions made by the ESM, rather than just using that data for initializing a prediction run. In addition to Earth system prediction, transfer operators can also be used for physics-based representation learning to extract coherent structures from simulation data produced by ESMs. For example, Fig 5. in [11] shows ocean gyres identified using transfer operators and Fig. 4 in [12] shows a data-driven decomposition of the TMQ field in the CAM5.1 model (there are updated but currently unpublished results that extract hurricanes from this data). Ref. [13] uses transfer operators to identify blocking events and provide an early-warning system.

Formally, rather than thinking of X as a collection of instrument readings, now think of X as abstractly representing a coherent structure, and we wish to use transfer operators to help identify and even define what X actually is in data. Typically, coherent structures are defined empirically, most often through orthogonal decomposition [14]. In the fluid dynamics community this is known as Proper Orthogonal Decomposition (POD), and Empirical Orthogonal Functions (EOFs) in the climate community. These methods attempt to identify coherent structures using linear features in the data. Transfer operators can capture nonlinear features that are physically motivated in terms of “almost-invariant sets”. From a Lagrangian perspective, this intuitively defines coherent structures as sets of points in the flow that tend to stay near one another over time. This approach has been used successfully to identify coherent structures relevant to the water cycle [11], [13], [15].

Further development and deployment of these transfer operator approaches to coherent structure detection will provide automated yet principled methods for identifying extreme events of the water cycle in the enormous data sets produced by E3SM. Ensemble studies are currently used to model the effect of various forcing scenarios on the Earth system. Such studies produce 10s to 100s of TB of data that must subsequently be analyzed, and simple summary statistics are insufficient for understanding the effects on extreme events in these studies. How will hurricane frequency and intensity change? Will their typical trajectories change? These and similar questions for other events like atmospheric rivers and blocking events require the automated identification of such events in simulation data. Supervised deep learning methods are the standard in computer vision, and have been applied to detect extreme weather events [16]. This approach requires training data with “ground-truth” labels, which is provided by automated thresholding heuristics [17]. Thus the neural network is really just learning these heuristics. In contrast, the transfer operator approach, as described above, provides an unsupervised physics-based alternative to defining the ground truth for coherent structures.

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